Electronic Theory of Solids
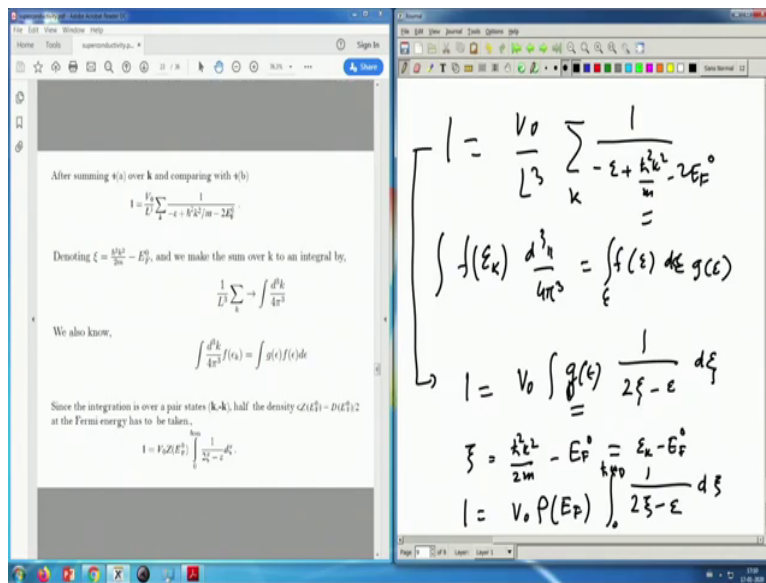**Prof. Arghya Taraphder**
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Lecture – 52
BCS Theory Introduction

So, we are almost towards the end of Coopers problem, so famous cooper problem.

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And we got this relation that 1 is equal to V 0 by L cube sum over k 1 by minus epsilon plus h cross square k square by m minus 2 E F 0 and we converted that that to an energy integral using this well known relations. Because this function for example, is a function of just this original the original energies, this the energy of the non interacting free electron. This is the free electron energy of basically 2 particles and so, this is a function of this original epsilon k.

So, as I wrote down that any integral of this kind over k. So, there you have d 3 k by 4 pi cube can be; d 3 k by 4 pi cube can be converted to a density of states integral. We which is epsilon, d epsilon, g of epsilon; where, g of epsilon is the density of states ok, of the original particles. So, that is the fermi c ok.

So that means, this equation now becomes 1 equal to V 0 g of e sorry g of E 1 by twice c minus epsilon and d of c ok; where, c is defined as h cross square k square by twice m which is epsilon k minus E F 0 is epsilon k minus E F 0 right. This epsilon k are the original energies of the original fermions electrons.

So, this is. So, I do something that I we have been doing all along is that since we are interested in the in a narrow region about the Fermi level and this can be taken. See this integral has to be within that h cross omega Debye window. So, this can be now taken outside by replacing it by its Fermi level value. So that means, that I can write this as V 0 Z E F sorry the V 0 the convention we are following is rho E F into integral over 1 by twice c minus epsilon d c 0 to h cross omega Debye. So, that is now achieved.

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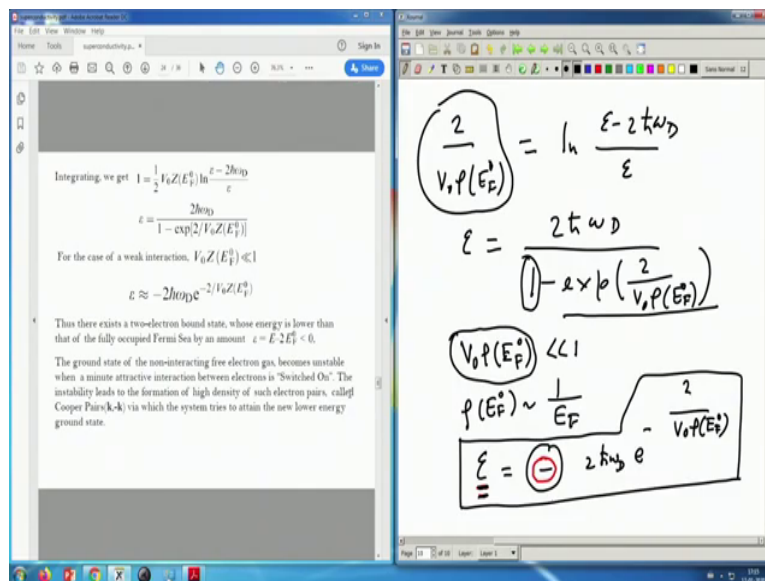
So, now the life our life is much simpler, all you have to do is to this integral which is straightforward which is which gives you this and so there is a logarithmic term. This logarithm will give you this result that you see the once you have this. So, let me just write down this result. So, 2 by V 0 rho E F equal to log of epsilon minus 2 h cross omega D divide by epsilon and that means, that epsilon is equal to 2 h cross omega D divided by 1 minus exponential of this quantity.

So, this I will just exponent your exponent it exponentiate it to get this 2 by V 0 rho E F ok. And that means, this E F 0 is of course, the same I am using E F 0. So, let me put E F 0 here that is the non interacting Fermi level energy of the Fermi level, Fermi energy and the original Fermi sea Fermi energy of the original Fermi sea

And that now what I can do is that since V 0 times rho E F effective, rho at Fermi level is much much less than 1; why? Because you see rho of E F is generally usually of order 1 by E F and then, V 0 is a very very tiny interaction that it was generated by that detailed process that we have discussed.

So, V 0 divided by E F is the scale of this object and this has to be very very small. E F being say 10000, 20000 degree Kelvin or 1 or 2 E V and V 0 is milli electron volt order. So, there is no comparison. So, you can just keep only 1 part of the exponential and then, the E to the power the other part you can replace by E to the power 0.

So, this sorry about it. What I am saying is that if you can look at it this is much larger and this much larger energy exponent can just be this 1 can just be ignored and this 1 is tiny number compared to this exponential 2 by V 0 rho E F. So, that is why we will just keep this exponential this; neglect the 1 and the result that you will get is epsilon equal to minus 2 h cross omega D e to the power minus 2 by V 0 rho E F and that is this result and the important thing is that this sign. So, this sign is what we what tells us that there is a negative value for epsilon.

So, epsilon turning out negative means that you have a state 2 particle energy state is actually below the Fermi level now. So, the 2 particles which were there, some of their energies were 2 E F naught has now come below the Fermi level, their combined energy is actually stabilized. So, the original energy and the new energies amongst them the new one is the lower energy.

So, this is really remarkable; this problem tells you that in the presence of a Fermi surface which blocks these states below it which are all filled up if you put 2 electrons just above this Fermi surface, these 2 electrons are allowed to interact by this retarded interaction which is attractive. Then, you will produce a bound state who is in total energy is less than the 2 E F,

not that the original energy was. So, this is a remarkable calculation in the sense that it opens the path for finding out the full theory of the superconductors which is what we will now go to ok.

So, that means, the now it says the ground state of the non interacting free electron gas becomes unstable, when a minute attractive interaction between electrons is switched on. So, this is this is an instability of the Fermi surface because the original Fermi surface was all the electrons fill up to up to E F E F naught. But now it shows that if you just put 2 electrons right above the Fermi surface, their total energy such that they will the bound state will form below the Fermi surface.

So that means, the Fermi surface, we start becoming unstable and that say it just indicates that you the or ground state is no longer a stable ground state. You have to look for a new ground state and probably there is a phase transition to a new ground state. So, that is what this theory of BCS undertook to explain starting from this kind of an idea that the Fermi surface has now become unstable.

You have to look for a new many body state which incorporates the idea of cooper that electrons pair up and that kind of a ground state was written down by Bob Schieffer and Robert Schrieffer and he and then, three of them combined to produce this extraordinary theory which is what I will study now.

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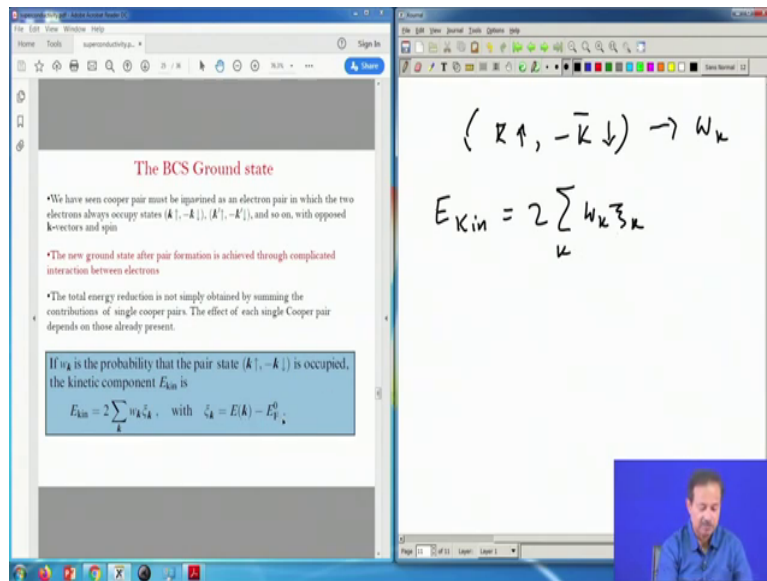
So, let us see ok. So, Cooper pair must be imagine as a as 2 electrons occupying state k up minus k down k prime up minus k prime down and so on right with their k vectors opposite and spins are also opposite. So, the trouble is that now you have to consider all the other 10 to the power 23 electrons that are in between these electrons, that are all there. So, it is a big soup of 10 to the power 23 electrons, they are interacting with each other and with these pairs and in between the these electrons which are just out of the Fermi level, they are trying to pair up. So, this is a mess of course.

But the basic idea is already laid down and what BCS did was that they realized that you just cannot sum up these negatives, minus epsilon energies to get the new energy. That is not what is happening. It is not a sum of all these 2 particle states is not just a product of these 2 particle states so that the energy is just the sum of this cooper bound state energy. That is not the case; you have to be able to write the full many body Hamiltonian and solve it in any way you can and that is what they undertook to do and the way they did it is just that, they wrote down a wave function for the many body states and that is what we are doing.

So, let us just go about looking at this is the suppose wk is the probability that the pair state k up minus k down is occupied ok. So, that probability is wk then its energy is of course e kinetic is equal to twice wk ck; where, c k is just some E k minus E F naught.

So, then there are these total energy reduction will happen and happen due to these scattering processes as we just saw k up minus k down going to k prime up minus k prime down states ok. And there are zillions and zillions of such scattering going on and the total energy will get lowered. So, what they wrote down was that they wrote down a wave function which is like this is u k times 0 plus v k times this 1; 0 k 1 k. What does the 0 k on 1 k mean? 0 k means state where the pair is unoccupied; 1 k means a pair state with the where the pair is occupied right.

So, and u k is; so, v k is the probability of occupying a state k up k down which is what we have written down wk square. So, this is the problem this is sorry, v k square is equal to the probability w k. Sorry about it. Because we define wk as the probability. So, v k square must be the probability w k and then, u k is the probability of singly occupied no occupation of that pair state.

So that means, u k square then must be equal to 1 minus v k square ok. So, that is so that is what this state defines. Now, one just takes a product of all such states. All such paired states for all such pairs momenta k and minus k. So, the BCS wave function, then is just a product of this kind of a wave function. It is called it is a pair, I mean it is just a very simple wave

function a pair being occupied with probability v k square and if pair being unoccupied with pair with probability u k square and such states are now taken product off.

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So, the BCS state that they predicted is pi over k product over all such k states u k 0 k plus v k 1 k, so that is it. So, this is the famous BCS state and it worked and that is the beauty of it that it produced a results which are marvelous which agreed with most of the experimental results of that time and for old superconductors, this really works extremely well.

So, that is what we are going to now work out. We will find out starting from this kind of a state how the physical properties different physical properties can be worked out and matched with the experimental values, experimental results. So, one can take a representation as 1 k is equal to 1, 0. We can write down a basis function like this because it is a 2 level system just to two things I mean a level can be occupied or unoccupied.

So, if it is unoccupied, its energy is 0. If it is occupied, its energy is whatever we had given c k. So, twice that 2 c k. So, that is that means, I again write down this these such things can always be represented by a by this even is a 2 by in the basis has 2 states. So, I can always represent by this way and such states can be then represented by a spin model actually, corresponding which makes transition between these 2 states which happens when a

scattering takes place by v k k prime and the 0 k state is 0, 1. So, this is my convention. This is how I define. This is the convention here used.

Now, you can transform these states between one another using Pauli matrices. These basically Pauli matrices can be used now to define a creation and annihilation operator which is half sigma k 1 sigma k 1 is given here plus i sigma k 2. So, sigma k 1 and sigma 2 are this these matrices. These are well known Pauli matrices and that is what that is that is being used here to write down this raising, so called raising operator. Now, what does it do? It basically changes a 0 occupation to a occupation 1. So, it will raises this number by 1 sigma minus is basically and sigma plus minus is basically this.

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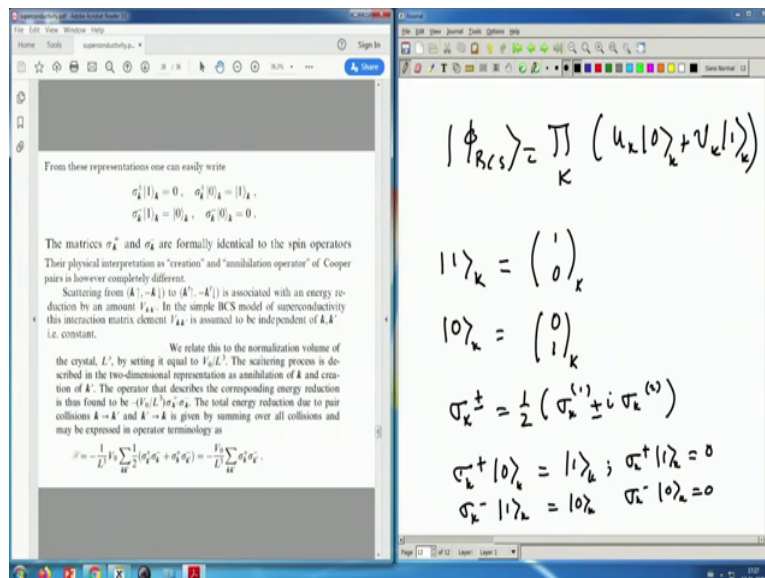
So, sigma the operations are then you can define sigma 1 sigma k plus operating on 0 k will give you 1 k; sigma k operating on 1 sigma k minus operating on 1 k will give you 0 k and sigma k plus operating on 1 k will give you 0.

Similarly, sigma k minus operating on 0 k will also give you 0. Because you cannot raise it beyond 1; you cannot raise you can cannot take 0 below it ok, the 0 state. So, these are things we have done several times in Heisen model also and Heisenberg model and so on. And in

simple harmonic oscillator also we have defined this raising lowering operators. But these are spin these are like pseudo spins, one can define this 1 and 0 as up and down spin if you like.

So, they are formally identical to the spin operators ok. So, they are basically creation and annihilation operator of cooper pairs ok. Then of course, the interpretation is very very different. They are basically creation and annihilation operator for cooper pairs, but they are formally identical to the spin operators that we have used many times ok.

So, as I said the scattering between the k up minus k down from one particular k paired state at k; that means, k and minus k occupied to another state which is k prime and minus k prime occupied is done via the v k k prime. So, the Hamiltonian should also reflect that as it did in the in this cooper problem as well. So, all that can be done here using these operators and this is exactly what this operator does. This operator basically destroys a state in here for example, if you look at this the state half sigma k prime plus sigma k minus; what does it do? It just destroys a pair at k annihilates a pair at k momentum; that means, k minus k and it creates a pair at k prime which minus k k prime minus k prime is now occupied and this is the Hermitian conjugate of that.

So, that is basically and then since you can again use k and k prime being different, you can use the matrix algebra and commute them and you will land up with this just one of them is good enough this is what we did in Heisenberg ferromagnetic remember. There we took the plus k on the right hand side, here we do not need to do that. So, this is how it is written. So, sigma plus k sigma minus k prime times v naught by L q of course, somewhere all such kk primes is the interaction term that represents the scattering.
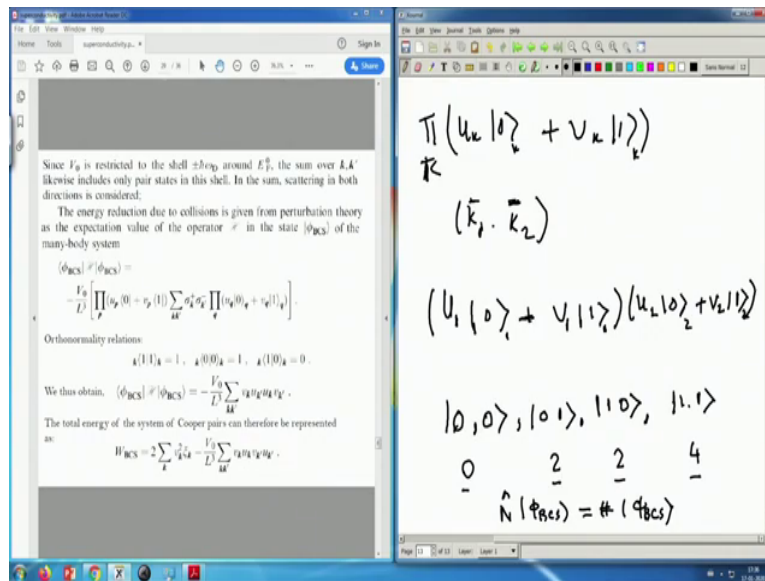
Again, remember that this V not we have to restrict and V not has to be restricted again within the shell of h cross omega D y because V not cannot work all over the band and over the entire fermi, all the states below the Fermi level. It only acts in a narrow strip around theFermi level and that restriction we have to again keep in mind while doing the integration, summations. Wherever kk prime summations come in, we have to remember the corresponding pairs energy must be within that the electrons that originally form the pair that their energies must be in that range. So, that is a restriction we have to keep in mind ok.

So, the energy reduction due to collision is now obtained by just a first order perturbation theory. Again, the V naught being so small compared to other energy scales in the system, one can just do a perturbation theory and that perturbation theory leads to this kind of a terms psi BCS h; psi BCS is simply this; this you can work out. This is very simple. Just take a take this kind of a product between 2 states to BCS states and you will get this absolutely straightforward.

And therefore, the total BCS energy total energy has to be summed over all such case. This is the first term we already wrote the kinetic energy and this is the second term is the term coming from scattering, taking kk k pair state to k prime pair scale pair state and vice versa and all such kk primes ok. So, that gives you this second term.

Now, one interesting thing about BCS wave function that it would like you to notice is that if you look at this wave function $u_k 0$ plus $v_k 1_k \pi$ over k, now if you just let us take a look aside and we I just want you to see what this wave function does. So, let us just assume that there are only 2 k states, so k_1, k_1 and k_2. So, these so that means, this is u_{k_1}. So, let me just not write k_1, k_2 let just write 1 which means u_{k_1} to make notation life simple, I will just write u_1 into 0 plus v_1 1 into u_2 0 plus v_2 1.

So, this is in one state; 1, this is in 2 ok. Now, let us look at it this first product is giving me u_1 into u_2 into two 0s. So, it says that both k_1 and k_2 pair states are unoccupied ok. So, let me just write this as; so both k_1 k_2 states are unoccupied this is the first term with u_1 into u_2. Second is u_1 into v_2, so the first state is unoccupied, but the second state is occupied. So, this has this is a this is a state with 2 electrons which amplitude is u_1 into v_2.

Similarly, v_1 into u_2 will have the similar which is 1 occupied and 2 unoccupied right. It has 2 electrons again. But then look at this last state product v_1, v_2 1, 1; 1, 1 this has 4 electrons. So, this is a 0 electron state; this is a 2 electron state; this is a 2 electron state; this is a 4 electron state. This means this is this is 0 pair, 1 pair, 1 pair, 2 pairs.

So, this wave function is actually a sum of all even number of electron states of this kind. So, you have you cannot have a single electron in this odd number of electrons are not and also the number of electrons in this state is not fixed. This state is a linear combination of 0, 2, 2, 4 electronic states. So, this is a remarkable state normally we are used to working with a fixed number of states, fixed number of electrons and this ground state that Bardeen Cooper and Schrieffer wrote down does not obey that. So, number is not a conserved quantity in this wave function, so number is no longer a good quantum number.

So, this wave function you should carefully handle that this wave function does not conserve the number and you have to fix the number by other means which is by using a Lagrange multiplier which is like a chemical potential and so on. So, that is an aside which I wanted to show you and want you to remember that this is a unique wave function which is not an eigen state.

So, if I try to find out by number operator operating on psi BCS, I will not get something here times psi BCS ok. So, it is not an eigen state of the number operator. So, that is something you have to you should remember and keep it in your mind that this is a very very different state from what we are used to in our normal quantum mechanics of many particle systems. There we are told that you have 2 particles or you have 5 particles or you have 10 particles or you have whatever particles and you write down the corresponding state by taking that many products and so on.

But here that prescription is not a not allowed, you are not doing that. You have you are doing something very very different and this is why this state is so unique, which we will discuss; the consequences of this we will discuss in the next class.